ION DISCLOSURE STATEMENT

ATTY. DOCKET NO. 1503.0200006

APPLICATION TO:

APPLICANT Agrafiotis et al.

FILING DATE March 12, 2001

GROUP 2123 FCH LEWIER 1600/2900

									41ER 1600/20
				U.S. P	ATEN	T DOCUMENTS			
EXAMINER INITIAL		DOCUMENT NUMBER	DAT	E	NAM	Е	CLASS	SUB- CLASS	FILING DATE
AK	AA1	4,773,099	09/1	988	Boks	er	382	14	
710	AB1	4,811,217	03/1	989	Tokiz	ane et al.	364	300	6 -
	AC1	4,859,736	08/1	989	Rink		525	54.1	
	AD1	4,908,773	03/1	990	Pante	oliano et al.	364	496	
	AE1	4,935,875	06/1	990	Shah	et al.	364		
	AF1	4,939,666	07/1		Hard		364	496	0 2
	AG1	5,010,175	04/1		1	er et al.	530	334	
	AH1	5,025,388	06/1			ner, III et al.	364	496	2002 9nter
1	Al1	5,155,801	10/1		Linco		395	22	12 (
	1701	10,100,001	1 10/1			ENT DOCUMENTS	1000		8
XAMINER NITIAL		DOCUMENT	NUMBER	DATE		COUNTRY	CLASS	SUB- CLASS	TRANSLATIO
AB	AJ1	EP 0 355 266	3 B1	02/1990		EPO	B01J	19/00	,
1	AK1	EP 0 355 628	3 B1	02/1990		EPO	G21F	9/00	
	AL1	EP 0 770 876	6 A1	05/1997		EPO	G01N	33/68	,
 MR	AM1	EP 0 818 744 Borg, II in Stati	OTHER (In		rick, M	itle, Date, Pertinent Pa		17/50	s, Springer Serie
↓ AB		Borg, li	OTHER (In	cluding Aut Groenen, Pat entire book	rick, <i>M</i> submitt	itle, Date, Pertinent Pa lodern Multidimensional led.	AUG 1 5 20	Application	s, Springer Serie
AB		Borg, In in Stati	OTHER (In	cluding Aut Groenen, Pat entire book s	rick, <i>M</i> submitt	itle, Date, Pertinent Pa	AUG 1 5 20	Application	s, Springer Seri
AB	AN	1 Borg, In in Stati	other (In angwer and Costics, 1997, tis, D.K. et a Academic Fortis, D.K. and Trees," J. Co	cluding Aut Groenen, Pat entire book s al., "Advance Publishers, V	es in div	itle, Date, Pertinent Pa	AUG 1 5 20 Sechnology Center in the property of Distance-Base	2) pplication 22 27 2100 29 2100 20 20 20 20 20 20 20 20	s, Springer Serional
MS	AO	1 Borg, II in Stati Agrafio Kluwer Agrafio on k-d pp. 51-	other (In angwer and Costics, 1997, Itis, D.K. et and Academic Formers," J. Cost. St.	cluding Aut Groenen, Pat entire book s al., "Advance Publishers, V d Lobanov, V them. Inf. Co.	es in div	itle, Date, Pertinent Parallel odern Multidimensional ted. versity profiling and con 999, pp. 1-22.	AUG 1 5 20 Cechnology Center of Distance-Base of Society, Vol. 39, If the Diversity And Queen Diversity A	22100 er 2100 esign," <i>Molec</i> eed Diveristy No. 1, Januar	s, Springer Serional
AB	AN AO	1 Borg, II in Stati Agrafio Kluwer Agrafio on k-d' pp. 51- Agrafio 1: 215t	other (In angwer and Costics, 1997, Itis, D.K. et a Academic Formation of the Academic Formation of the Acs Nation of th	cluding Autorian Comments of Lobanov, Vonal Meeting, de Jaeger, E.F.	es in divol. 4, 1 /.S., "A /.S., "B /.S., "Dire	lodern Multidimensional ted. Versity profiling and con 999, pp. 1-22. In Efficient Implementat Sci., American Chemical tridging The Gap Between the profile of the profil	AUG 1 5 20 AUG 1 5 20 Technology Center of the control of Distance-Basel Society, Vol. 39, Incomplete the complete the control of the contr	pplication 2 2 2100 esign," Molecular sed Diveristy No. 1, Januar SAR," Abstra	s, Springer Series Fular Diversity, Measures Basery/February 1999 Cts of Papers Pa

ANG 0 9 SOUS									Page 2 of 36
						TY. DOCKET NO. 03.0200006		CATION NO 02,956	CEIVE
THE THE PERSON	<i>\$</i>		PTO-1449 CLOSURE STATE	EMENT	AF	PLICANT rafiotis et al.		A	UG 1 4 2002
TO THE						LING DATE arch 12, 2001	GROUI 2123	? TECH C	ENTER 1600/2
				U.S		T DOCUMENTS		· · · · · · · · · · · · · · · · · · ·	**************************************
XAMINER NITIAL				DATE	NAM	1E	CLASS	SUB-	FILING DATE
NAR -	AA2	† —	IBER 1	1/1992	Skei	rile	395	CLASS 27	
LXID	AB2	+		1/1992	Rorv		382		\$ 77
	AC2	+	.,)8/1993		kermann et al.	422	67	D
	AD2	+		11/1993 11/1993 12/1993		co et al.	364	499	
—	AE2	+				nick et al.	364	496	
	AF2	+					435	727	b 22 111
	AG2	 		2/1994	Schatz et al.		427	2 =	4
1.	AH2		<u> </u>	04/1994	-	ner, III et al.	364	1 400	1 8 m
4	Al2			06/1994	Haya		382	15	
- -	7	0,02				PATENT DOCUMENTS			
AMINER TIAL		DOC	CUMENT NUMBE			COUNTRY	CLASS	SUB-	TRANSLATION
Ars	AJ2	wo	WO 91/19735 12/1991		91 PCT		C07K	7/02	Yes No
	AK2	wo.	O_92/00091 01/1992			PCT	A61K	37/02	Yes No
	AL2	wo	93/20242	0242 10/1993		РСТ .	C12Q	1/70	Yes No
V	AM2	wo	94/28504	12/1994	ļ	PCT	G06F	15/60	Yes
							l	i	No
	T 1		OTHER	(Including A	Author, T	L itle, Date, Pertinent Pages	s, etc.)	<u> </u>	I NO
AB .	AN	2		, "Diversity of	Chemica	I itle, Date, Pertinent Pages al Libraries," <i>Encyclopedia d</i>		_	
AB	AO	2	Agrafiotis, D.K., Ltd, Vol. 1:A-D, Agrafiotis, D.K.,	, "Diversity of 1998, pp. 74 , "On the Use	Chemica 2-761.		AUG 1 5 2	2002	ohn Wiley & Sons
AB			Agrafiotis, D.K., Ltd, Vol. 1:A-D, Agrafiotis, D.K., Sci., American	, "Diversity of 1998, pp. 74 , "On the Use Chemical Soc et al., "Parall	Chemica 2-761. of Infornciety, Vol	al Libraries," <i>Encyclopedia o</i>	AUG 1 5 2 echnology Cer Molecular Diver pp. 576-580.	2002 Inter 2100 Sity," <i>J. Cher</i>	ohn Wiley & Sons
AB	AO	<u>2</u>	Agrafiotis, D.K., Ltd, Vol. 1:A-D, Agrafiotis, D.K., Sci., American Agrafiotis, D.K. 1999, p. 50-CO	, "Diversity of 1998, pp. 74 , "On the Use Chemical Soc et al., "Parall MP.	Chemica 2-761. of Inforn ciety, Vol	nation Theory for Assessing	AUG 1 5 2 echnology Cer Molecular Diver pp. 576-580. 1: 217th ACS Na	2002 Ater 2100 rsity," J. Cher ational Meetin	ohn Wiley & Sons m. Inf. Comput. ng, March 21-25,
AB	AO	2	Agrafiotis, D.K., Ltd, Vol. 1:A-D, Agrafiotis, D.K., Sci., American Agrafiotis, D.K. 1999, p. 50-CO Agrafiotis, D.K. Computational	, "Diversity of 1998, pp. 74 , "On the Use Chemical Societ al., "Parall MP. et al., "PROLChemistry, Journal Jaeger, 1998, pp.	Chemica 2-761. of Inform ciety, Vol el QSAR DEN: A N phn Wiley	nation Theory for Assessing 37, No. 3, May/June 1997, "Abstracts of Papers Part	AUG 1 5 2 echnology Cer Molecular Diver pp. 576-580. 1: 217th ACS Na Integrated Proje 9, October 1990,	ected Populati	ohn Wiley & Sons m. Inf. Comput. ag, March 21-25, ions," Journal of

ATTY. DOCKET NO. 1503.0200006 APPLICATION 09/802,956 AUG 1 4 2002 FORM PTO-1449 APPLICANT Agrafiotis et al. ION DISCLOSURE STATEMENT TECH CENTER 1600/2900 GROUP FILING DATE March 12, 2001 2123 **U.S. PATENT DOCUMENTS EXAMINER** CLASS SUB-FILING DATE INITIAL DOCUMENT DATE NAME **CLASS** NUMBER AA3 07/1994 364 500 k 5,331,573 Balaji et al. 364 496 АВ3 5,434,796 07/1995 Weininger AC3 Eisenberg et al. 364 496 5,436,850 07/1995 Noda et al. 564 426 AD3 5,442,122 08/1995 AE3 5,463,564 Agrafiotis et al. 364 496 10/1995 364 500 03/1996 Sugawara et al. AF3 5,499,193 AG3 5,519,635 05/1996 Miyake et al. 364 497 **АНЗ** 06/1996 Yagasaki 382 226 5,524,065 AI3 5,526,281 06/1996 Chapman et al. 364 496 **FOREIGN PATENT DOCUMENTS EXAMINER** DOCUMENT NUMBER COUNTRY SUB-TRANSLATION INITIAL DATE CLASS **CLASS** 01/1995 **PCT** G06F 15/42 AJ3 WO 95/01606 Yes No PCT C07H 21/02 Yes АК3 WO 97/09342 03/1997 No AL3 WO 97/20952 PCT C12Q 1/68 Yes 06/1997 No АМЗ WO 97/27559 07/1997 PCT G06F 19/00 Yes No OTHER (Including Author, Title, Date, Pertinent Pages, etc.) Agrafiotis, D., "Theoretical Aspects of the Complex: Arts and New Technological Application Impacts AN 3 Information Processing '94, North-Holland, Vol. II, 1994, pp. 714-719. AUG 1 5 2002 Technology Center 2100
Biswas, G. et al., "Evaluation of Projection Algorithms," IEEE Transactions On Pattern Analysis And Machine AO 3 Intelligence, IEEE Computer Society, Vol. PAMI-3, No. 6, November 1981, pp. 701-708. Bonchev, D. and Trinajstić, N., "Information theory, distance matrix, and molecular branching," *The Journal of Chemical Physics*, American Institute of Physics, Vol. 67, No. 10, November 15, 1977, pp. 4517-4533. AP 3 Chang, C.L. and Lee, R.C.T., "A Heuristic Relaxation Method for Nonlinear Mapping in Cluster Analysis," IEEE Transactions on Systems, Man, and Cybernetics, IEEE Systems, Man, and Cybernetics Society, Vol. SMC-3, AQ <u>3</u> March 1973, pp. 197-200.

EXAMINER Jamuelly 12/03/03

EXAMINER: Initial if reference considered, whether or not citation is in conformance with MPEP 609. Draw line through citation if not in conformance and not considered. Include copy of this form with next communication to Applicant.

Cramer, R.D. et al., "Virtual Compound Libraries: A New Approach to Decision Making in Molecular Discovery Research," J. Chem. Inf. Comput. Sci., American Chemical Society, Vol. 38, No. 6, November/December 1998,

AR

3

pp. 1010-1023.

Page 4 of 36 APPLICATION NO. ATTY. DOCKET NO. 1503.0200006 09/802,956 FORM PTO-1449 APPLICANT Agrafiotis et al. MATION DISCLOSURE STATEMENT GROUP FILING DATE March 12, 2001 2123 **U.S. PATENT DOCUMENTS EXAMINER** SUB-INITIAL DOCUMENT NAME **CLASS** FILING DATE DATE **CLASS** NUMBER 436 518 AA4 5,545,568 08/1996 Ellman Œ Holmes 428 403 AB4 5,549,974 08/1996 Perry TECH CENTER 1600/290995 157 AC4 5,553,225 09/1996 435 7.1 AD4 Blake 5,565,325 10/1996 AE4 364 500 5,574,656 11/1996 Agrafiotis et al. Bowie et al. 436 518 AF4 5,585,277 12/1996 AG4 5,602,755 Ashe et al. 364 498 02/1997 382 155 AH4 5,602,938 02/1997 Akiyama et al. Al4 5,612,895 03/1997 Balaji et al. 364 496 **FOREIGN PATENT DOCUMENTS EXAMINER** INITIAL **DOCUMENT NUMBER** DATE COUNTRY **CLASS** SUB-TRANSLATION **CLASS** PCT G06F 17/50 AJ4 WO 98/20437 05/1998 Yes No RECEIVED PCT G06T AK4 WO 98/20459 05/1998 11/20 Yes No AUG 1 5 2002 AL4 Yes No AM4 Yes **Technology Center 2100** No OTHER (Including Author, Title, Date, Pertinent Pages, etc.) AN 4 Systems, Vol. 5, 1993, pp. 580-587.

DeMers, D. and Cottrell, G., "Non-Linear Dimensionality Reduction," Advances in Neural Information Processing Frey, P.W. and Slate, D.J., "Letter Recognition Using Holland-Style Adaptive Classifiers," Machine Learning, AO 4 Kluwer Academic Publishers, Vol. 6, 1991, pp. 161-182. Friedman, J.H., "Exploratory Projection Pursuit," Journal of the American Statistical Association, American AP 4 Statistical Association, Vol. 82, No. 397, March 1987, pp. 249-266. Friedman, J.H. and Tukey, J.W., "A Projection Pursuit Algorithm for Exploratory Data Analysis," IEEE AQ 4 Transactions on Computers, IEEE Computer Society, Vol. C-23, No. 9, September 1974, pp. 881-889. Garrido, L. et al., "Use of Multilayer Feedforward Neural Nets As A Display Method for Multidimensional Distributions," International Journal of Neural Systems, World Scientific Publishing Co. Pte. Ltd., Vol. 6, No. 3, AR 4 September 1995, pp. 273-282.

EXAMINER

DATE CONSIDERED

ATTY. DOCKET NO. 1503.0200006 APPLICAT 09/802 9 FORM PTO-1449 APPLICANT Agrafiotis et al. TION DISCLOSURE STATEMENT FILING DATE GROUP March 12, 2001 2123**T U.S. PATENT DOCUMENTS EXAMINER** INITIAL DATE NAME **CLASS** SUB-FILING DATE DOCUMENT CLASS NUMBER 05/1997 395 326 AA5 5,634,017 Mohanty et al. 334 530 AB5 5,635,598 06/1997 Lebl et al. 435 7.1 09/1997 Beutel AC5 5,670,326 436 518 10/1997 Bowie et al. AD5 5,679,582 11/1997 Agrafiotis et al. 364 500 AE5 5,684,711 364 496 Chapman AF5 5,703,792 12/1997 AG5 5,712,171 01/1998 Zambias et al. 436 518 324 210 AH₅ 01/1998 Hayosh 5,712,564 AI5 5,736,412 04/1998 Zambias et al. 436 518 **FOREIGN PATENT DOCUMENTS EXAMINER** COUNTRY CLASS SUB-INITIAL **DOCUMENT NUMBER** DATE TRANSLATION **CLASS** RECEIVED AJ5 Yes No AK5 Yes AUG 1 5 2002 No Yes AL5 Technology Center 2100 No AM5 Yes No OTHER (Including Author, Title, Date, Pertinent Pages, etc.) Ghose, A.K. et al., "Prediction of Hydrophobic (Lipophilic) Properties of Small Organic Molecules Using AN <u>5</u> Fragmental Methods: An Analysis of ALOGP and CLOGP Methods," J. Phys. Chem. A, American Chemical Society, Vol. 102, No. 21, May 21, 1998, pp. 3762-3772. Hall, L.H. and Kier, L.B., "The Molecular Connectivity Chi Indexes and Kappa Shape Indexes in Structure-AO 5 Property Modeling," Reviews in Computational Chemistry: Advances, VCH Publishers, Inc., 1991, pp. 367-422. Hecht-Nielsen, R., "Replicator Neural Networks for Universal Optimal Source Coding," Science, American AΡ <u>5</u> Association for the Advancement of Science, Vol. 269, September 29, 1995, pp. 1860-1863. Hotelling, H., "Analysis of a Complex of Statistical Variables into Principal Components," The Journal of AQ <u>5</u> Educational Psychology, Warwick and York, Inc., Vol. XXIV, No. 6, September 1933, pp. 417-441. Hotelling, H., "Analysis of a Complex of Statistical Variables into Principal Components," The Journal of AR <u>5</u> Educational Psychology, Warwick and York, Inc., Vol. XXIV, No. 7, October 1933, pp. 498-520.

EXAMINER: Initial if reference considered, whether or not citation is in conformance with MPEP 609. Draw line through citation if not in conformance and not considered. Include copy of this form with next communication to Applicant.

EXAMINER

6	PE	<u></u>										
♦ AU6	0 9 5005							TY. DOCKET NO).	APPLI 09/80		Page 6 of 36 CEIVEL
3	ۍ	F	ORM P	TO-1449			AP	APPLICANT AUG 1 4 20				
ANTAN 8	TRAIN	RMATIO	N DISC	CLOSURE STA	TEMEN	<u>IT</u>	Agrafiotis et al. FILING DATE March 12, 2001 GROUP TECH CENTER 160					
						U.S. P		DOCUMENTS		1,5255	100,	
EXAMII				:UMENT IBER	DATI		NAM			CLASS	SUB- CLASS	FILING DATE
1/2	1/3	AA6	5,74	0,326	04/19	98	Boule	et et al.		395	27	
		AB6	5,78	9,160	08/19	998	Eato	n et al.		435	6	
		AC6	5,80	7,754	09/19	98	Zaml	oias et al.		436	518	
	\	AD6	5,81	1,241	09/19	998	Good	fellow et al.		435	7.1	
	1	AE6	5,83	2,494	11/19	998	Egge	r et al.		707	102	
		AF6	5,85	8,660	01/19	999	Eato	n et al.		435	6	
		AG6	5,86	1,532	01/19	999	Brow	n et al.		564	142	
		AH6	5,86	6,334	02/19	999	Beute			435	6	
ļ	Υ	Al6	5,90	1,069	05/19	999	Agra	iotis et al.		364	528.03	
		·				FOREIGN	PATE	NT DOCUMENT	rs			-
EXAMII INITIAL			DOC	UMENT NUM	BER	DATE		COUNTRY	חרס	CLASS	SUB- CLASS	TRANSLATION
		AJ6			RE	CEIVE	D		HEC	EIVE	D	No
-		AK6			AU(1 5 200	02		AUG	1 2 2002		Yes No
		AL6		Те	chnol	ogy Center	r 210)	Technolog	y Center	2100	Yes No
		AM6										Yes No
				ОТН	ER (In	cluding Aut	hor, T	tle, Date, Pertin	ent Pages, etc	:.)		
A	K	AN	<u>6</u>					thod for the Sequential Institute of Elec				e to Two-Space," n 1977, pp. 288-
		AO	<u>6</u>	Lipinski, C.A. discovery and pp. 3-25.	et al., d deve	"Experimen lopment sett	tal and	computational a	pproaches to e Delivery Revieu	estimate solu vs, Elsevier	ubility and pe Science B.V	ermeability in drug /., Vol. 23, 1997,
		AP	<u>6</u>					telligent Databas 2, 1998, p. 19-C		niques," Abs	stracts of Pa	pers Part 1: 215th
		AQ	<u>6</u>	Lobanov, V.S <i>Meeting</i> , Mar					_ibraries," <i>Abst</i>	racts of Pap	ers Part 1: 2	217th ACS National

EXAMINER DATE CONSIDERED

Mao, J. and Jain, A.K., "Artificial Neural Networks for Feature Extraction and Multivariate Data Projection," *IEEE transactions on Neural Networks*, IEEE Neural Networks, Vol. 6, No. 2, March 1995, pp. 296-317.

EXAMINER: Initial if reference considered, whether or not citation is in conformance with MPEP 609. Draw line through citation if not in conformance and not considered. Include copy of this form with next communication to Applicant.

AR

<u>6</u>

INFORMATION DISCLOSURE STATEMENT

ATTY. DOCKET NO. 1503.0200006

APPLICATION NO

APPLICANT Agrafiotis et al.

					U.S. P		T DOCUMENTS		2123	TEUNU	<u>=₁↓↑EN 1600/2</u> 9
XAMINER			CUMENT MBER	DATE	Ξ	NAM	E		CLASS	SUB- CLASS	FILING DATE
MS	AA7		08,960	06/19	999	Newl	ander		564	177	
1	AB7	_	3,819	11/19			es et al.		424	188.1	
	AC7		4,661	01/20	000		erg et al.		707	3	
	AD7	_	37,135	03/20	000		et al.		435	7:24	
	AE7	6,04	19,797	04/20	000	Guha	ı et al.		707	6	
V	AF7	6,18	35,506 B1	02/20	001	Cram	er et al. /		702	19	
	AG7							*			
	AH7					<u> </u>				ļ	
	AI7	Ш		<u> </u>					<u> </u>	L .	<u> </u>
		$\overline{}$			FOREIGN	I PATE	ENT DOCUMENTS	S	i	<u> </u>	1
XAMINER NITIAL		DOC	CUMENT NUMI	BER	DATE		COUNTRY .		CLASS	SUB- CLASS	TRANSLATION
	AJ7				REC	ΕΙV	ED	RE	CEIV	ED	Yes No
	AK7				AUG	157	002	AL	G 1 2 20	02	No
	AL7				Technolog	y Cer	nter 2100	Techno	ogy Cent	er 2100	Yes No
	AM7			;							Yes
			ОТНІ	ER (Inc	l cluding Auti	hor, Ti	itle, Date, Pertine	nt Pages, et	C.)		No
MS	AN	7		cipal C	Components,	Minor	itie, Date, Pertine Components, and			' Neural Net	works, Pergamon
MS	AN	7	Oja, E., "Prin Press Ltd., V	icipal C	Components, 992, pp. 927	Minor 7-935.	Components, and	I Linear Neur	al Networks,	'Molecular	works, Pergamon
ANS			Oja, E., "Prin Press Ltd., V Patterson, D. Descriptors,"	cipal Col. 5, 1	Components, 1992, pp. 927	Minor 7-935. rhood I	Components, and	I Linear Neur	al Networks," Validation of ciety, Vol. 39	'Molecular , No. 16, 19	works, Pergamon Diversity' 96, pp. 3049-3059.
AB	AO	7	Oja, E., "Prin Press Ltd., V Patterson, D. Descriptors," Pykett, C.E., Electronics L	cipal Colors, 1 E. et al Journal "Impro- etters,	Components, 1992, pp. 927 al., "Neighbor al of Medicinal of Medicinal over the Institute an, P., "A See	Minor 7-935. rhood I nal Che	Components, and Behavior: A Useful emistry, American of Sammon's Nor	I Linear Neur I Concept for Chemical So Inlinear Mappi Vol. 14, No.	Validation of ciety, Vol. 39	'Molecular , No. 16, 19 Clustering A er 7, 1978, p	works, Pergamon Diversity' 96, pp. 3049-3059 archetypes," pp. 799-800.
AB	AO	Z	Oja, E., "Printeress Ltd., Volume Press Ltd., Volume Patterson, D. Descriptors," Pykett, C.E., Electronics L. Rubner, J. ar European Ph. Sadowski, J.	"E. et al.,	Components, 1992, pp. 927 al., "Neighbor al of Medicinal of Medicinal of Medicinal over the Institute an, P., "A Se Society, Vol. "Assessing statements of the Institute and Institute	Minor 7-935. rhood I nal Che	Components, and Behavior: A Useful emistry, American of Sammon's Nor ectrical Engineers,	I Linear Neur I Concept for Chemical So Inlinear Mappi Vol. 14, No.	Validation of ciety, Vol. 39 ng by Using 25, December 25, December 3-698.	Clustering Aer 7, 1978, p	Diversity' 96, pp. 3049-3059 archetypes," pp. 799-800.



INFORMATION DISCLOSURE STATEMENT

ATTY. DOCKET NO. 1503.0200006	APPLICATION NO. 09/802,956
APPLICANT Agrafiotis et al.	

· .							LING DATE rch 12, 2001		GROUP 2123		
					U.S. P	ATEN	T DOCUMENTS				
EXAMINER INITIAL			UMENT IBER	DAT	Ē	NAM	E		CLASS	SUB- CLASS	FILING DATE
	AA8						-OEIV	LU			
	AB8	ļ				<u> </u>	3Elini	.()))			
	AC8	-		ļ		•	AUG 1 4	<u> 200</u> ε			
	AD8	1					- NOCH	1900 5 300)		-
	AE8	+				7	ECH CENTER				
	AG8	 				<u> </u>					
	AH8										
	Al8				•						
					FOREIGN	PAT	ENT DOCUMENTS	S			
EXAMINER INITIAL		DOC	UMENT NUM	BER	DATE		COUNTRY		CLASS	SUB- CLASS	TRANSLATION
	AJ8				REC	ΈŅ	FD	RE	CEIV	ED	No
	AK8				AUG		_	Д	G 1 2 20	02	No
	AL8				Technolog			Techno	ogy Cent	er 2100	No
	AM8			,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,			<u></u>			Yes No	
			ОТН	ER (In	cluding Aut	hor, T	itle, Date, Pertine	nt Pages, e	tc.)		
Ms	AN	<u>8</u>	Thompson, L American Ch	A. and emical	d Ellman, J./ I Society, Vo	A., "Sy I. 96, I	nthesis and Applic No. 1, January/Feb	ations of Sm oruary 1996,	nall Molecule I pp. 555-600.	ibraries," <i>C</i>	hemical Reviews,
	AO	<u>8</u>					1 ., "Computer repri <i>esign</i> , Kluwer Aca				natorial libraries,"
	AP	<u>8</u>	Brint, Andrev chemical stru No. 4, Janua	ictures	," Journal of	Comp	pperbound proced uter-Aided Molecu	lures for the ular Design,	identification of ESCOM Scien	of similar thr nce Publishe	ee-dim nsional ers B.V., Vol. 2,
	AQ	8					C., "Designing Co can Chemical Soc				Genetic Algorithm," 2313.
	AR	<u>8</u>		ournal o			ess of Reactant Po ation Computer Sc				
EXAMINER	Am	nel	Brida						DATE CONS	DERED	

Page 9 of 36 ATTY. DOCKET NO. APPLICATION NO. 09/802,956 1503.0200006 FORM PTO-1449 APPLICANT Agrafiotis et al. RMATION DISCLOSURE STATEMENT GROUP FILING DATE March 12, 2001 2123 **U.S. PATENT DOCUMENTS EXAMINER** INITIAL DATE NAME **CLASS** SUB-**FILING DATE** DOCUMENT NUMBER CLASS AA9 AB9 AC9 AD9 AE9 AF9 AG9 AH9 AI9 FOREIGN PATENT DOCUMENTS **EXAMINER** COUNTRY DOCUMENT NUMBER DATE **CLASS** SUB-TRANSLATION INITIAL AJ9 Yes RECEIVED No AUG 1 2 2002 AK9 Yes AUG 1 5 2002 No Technology Center 2100 AL9 Yes No Technology Center 2100 AM9 Yes No OTHER (Including Author, Title, Date, Pertinent Pages, etc.) Gillet, Valerie J. et al., "Selecting Combinatorial Libraries to Optimize Diversity and Physical Properties," Journal AN 9 of Chemical Information Computer Sciences, American Chemical Society, Vol. 39, No. 1, 1999, pp. 169-177. Kearsley, Simon K. et al., "Chemical Similarity Using Physiochemical Property Descriptors," Journal of Chemical AO 9 Information Computer Science, American Chemical Society, Vol. 36, No. 1, 1996, pp. 118-127. Leland, Burton A. et al., "Managing the Combinatorial Explosion," Journal of Chemical Information Computer AP 9 Science, American Chemical Society, Vol. 37, No. 1, 1997, pp. 62-70. Lewis, Richard A. et al., "Similarity Measures for Rational Set Selection and Analysis of Combinatorial Libraries: AQ The Diverse Property-Derived (DPD) Approach," Journal of Chemical Information Computer Science, American 9 Chemical Society, Vol. 37, No. 3, 1997, pp. 599-614.

EXAMINER Jamulyydy DATE, CO. 12/03

EXAMINER: Initial if reference considered, whether or not citation is in conformance with MPEP 609. Draw line through citation if not in conformance and not considered. Include copy of this form with next communication to Applicant.

Martin, Eric J. and Critchlow, Roger E., "Beyond Mere Diversity: Tailoring Combinatorial Libraries for Drug

Discovery," Journal of Combinatorial Chemistry, American Chemical Society, Vol. 1, No. 1, 1999, pp. 32-45.

AR

9

Page 10 of 36 ATTY. DOCKET NO. 1503.0200006 APPLICATION NO. 09/802,956 FORM PTO-1449 APPLICANT Agrafiotis et al. ION DISCLOSURE STATEMENT FILING DATE GROUP March 12, 2001 2123 **U.S. PATENT DOCUMENTS EXAMINER** INITIAL DOCUMENT DATE NAME **CLASS** SUB-FILING DATE NUMBER CLASS AA10 AB10 AC10 AD10 AE10 AF10 AG10 AH10 AI10 **FOREIGN PATENT DOCUMENTS EXAMINER** COUNTRY **CLASS** TRANSLATION INITIAL DOCUMENT NUMBER DATE SUB-AJ10 Yes No AVG 1 2 ZVUZ AK10 Yes No Technology Center 2100 AL10 Yes No AM10 Yes No OTHER (Including Author, Title, Date, Pertinent Pages, etc.) Sheridan, Robert P. et al., "Chemical Similarity Using Geometric Atom Pair Descriptors," Journal of Chemical ΑN 10 Information Computer Science, American Chemical Society, Vol. 36, No. 1, 1996, pp. 128-136. Willett, Peter et al., "Chemical Similarity Searching," Journal of Chemical Information Computer Science, AO <u>10</u> American Chemical Society, Vol. 38, No. 6, 1998, pp. 983-996. Agrafiotis, Dimitris K. and Lobanov, Victor S., "Ultrafast Algorithm for Designing Focused Combinational Arrays," ΑP 10 J. Chem. Inf. Comput. Sci., American Chemical Society, 2000, Vol. 40, No. 4, pp. 1030-1038. Ajay et al., "Can We Learn To Distinguish between 'Drug-Like' and 'Nondrug-like' Molecules?" J. Med. Chem., AQ 10 1998, American Chemical Society, Vol. 41, No. 18, pp. 3314-3324. Brown, Robert D. and Martin, Yvonne C., "Designing Combinatorial Library Mixtures Using a Genetic Algorithm," AR 10 J. Med. Chem., American Chemical Society, 1997, Vol. 40, No. 15, pp. 2304-2313. **EXAMINER EXAMINER**: Initial if reference considered, whether or not citation is in conformance with MPEP 609. Draw line through citation if not in

conformance and not considered. Include copy of this form with next communication to Applicant.

Page 11 of 36 ATTY. DOCKET NO. 1503.0200006 APPLICATION NO. 09/802,956 FORM PTO-1449 APPLICANT Agrafiotis et al. TION DISCLOSURE STATEMENT GROUP FILING DATE March 12, 2001 2123 **U.S. PATENT DOCUMENTS EXAMINER** DATE **CLASS** FILING DATE DOCUMENT NAME SUB-INITIAL NUMBER **CLASS** AA11 AB11 AC11 AD11 AE11 4 AF11 CENTER 1000/2900 AG11 AH11 **AI11 FOREIGN PATENT DOCUMENTS EXAMINER** DOCUMENT NUMBER DATE COUNTRY CLASS SUB-INITIAL TRANSLATION **CLASS** AJ11 N/A RECEIVED AK11 Yes 2 2002 AUG 1 AUG 1 5 2002 (See AP50) AL11 Yes Technology Center 2100 Technology Center 2100 (See AR50) AM11 Yes (See AN51) OTHER (Including Author, Title, Date, Pertinent Pages, etc.) Brown, Robert D. and Martin, Yvonne C., "The Information Content of 2D and 3D Structural Descriptors ΑN <u>11</u> Relevant to Ligand-Receptor Binding," J. Chem. Info. Comput. Sci., American Chemical Society, 1997, Vol. 37, No. 1, pp. 1-9. Brown, Robert D. and Martin, Yvonne C., "Use of Structure-Activity Data To Compare Structure-Based Clustering Methods and Descriptors for Use in Compound Selection," J. Chem. Inf. Sci., American Chemical AO <u>11</u> Society, 1996, Vol. 36, No. 3, pp. 572-584. Cummins, David J. et al., "Molecular Diversity in Chemical Databases: Comparison of Medicinal Chemistry AΡ 11 Knowledge Bases and Databases of Commercially Available Compounds," J. Chem. Info. Comput. Sci., American Chemical Society, 1996, Vol. 36, No. 4, pp. 750-763. Daylight Theory: Fingerprints (visited September 26, 2000) AQ <u>11</u> http://www.daylight.com/dayhtml/doc/theory/theory.finger.html, 9 pages.

EXAMINER Janual Rush

Daylight Theory: SMARTS (visited September 26, 2000)

EXAMINER: Initial if reference considered, whether or not citation is in conformance with MPEP 609. Draw line through citation if not in conformance and not considered. Include copy of this form with next communication to Applicant.

+ 10 pages.

AR

<u>11</u>

101FE									P	age 12 of 36
(AUG 0 9 2007							TY. DOCKET NO.	APPLI 09/80	CAT ON NO.	
9.	ste E		PTO-1449			AP	PLICANT rafiotis et al.			G 1 4 2002
THANKS THE THE	ØRMATIOI	1 DIS	CLOSURE STAT	'EMEN	<u>IT</u>	FI	LING DATE	GROUP		NIER 1600/290
					IIS P		rch 12, 2001 DOCUMENTS	2123	TEOU OF	NIER 1800/290
EXAMINER INITIAL		DOC	CUMENT	DATE		NAM		CLASS	SUB-	FILING DATE
	AA12	NUM	MBER						CLASS	
	AB12									
	AC12	 								
	AD12	1					RE	CEN	/ED	
	AE12	1								
	AF12						A	JG 1 2 2	002	
	AG12	1							T	
	AH12						- recnnq	logy Cen	er 2100	
	Al12	†	i						,	
					FOREIGN	PATE	ENT DOCUMENTS		•	•
EXAMINER INITIAL		DOC	CUMENT NUMB	ER	DATE		COUNTRIRECEIVED	CLASS	SUB- CLASS	TRANSLATION
	AJ12						N			
	AK12						AUG 1 5 2002			
	AL12						Technology Center 21			
	AM12						ocine, 2	00		
		·	OTHE	R (Inc	cluding Autl	hor, Ti	tle, Date, Pertinent Pages, etc	.)		
Ms	AN	<u>12</u>					I., "Techniques for Generating D American Chemical Society, 199			
	AO	<u>12</u>	Gillet, Valerie Academic Pub				of Molecular Diversity," <i>Molecul</i> a	ar Diversity	in Drug Desi	<i>gn</i> , Kluwer
	АР	<u>12</u>		Up t	he Design P		A., "New Methodology for Profilir s with HARPick," <i>J. Med. Chem.</i> ,			
	AQ .	<u>12</u>					, "Functional diversity of compou 000, Vol. 4, No. 3, pp. 287-294.	und libraries	," Current op	inion in chemical
	AR	<u>12</u>					eagent-Based and Product-Base em. Inf. Comput. Sci., American			
EXAMINER	Sa	mu	Muda				D	ATE CONS	DERED	
	nitial if refe	rence	considered, whe				conformance with MPEP 609. In mmunication to Applicant.		_	if not in

ATTY. DOCKET NO.

APPLICATION NO.

EXAMINER NITIAL			TO-1449	TEMEN	<u>rr</u>		PLICANT rafiotis et al.	09/80		
EXAMINER	ORMATIO	N DISC	CLOSURE STA	TEMEN	<u>IT</u>	Ag	railotis et al.		•	
			* *			FT	LING DATE	GROUP		
						Ma	rch 12, 2001	2123	·	
				r	U.S. P	ATEN	T DOCUMENTS	1	Γ	<u> </u>
	DOCUMENT DATE NUMBER AA13				E	NAM	E	CLASS	SUB- CLASS	FILING DATE
	AA13	<u> </u>								
	AB13		· · · · · · · · · · · · · · · · · · ·					hee e	IN/EF	
	AC13	<u> </u>						RECE	IIVEL	,
	AD13			<u> </u>				Aug 1	2 2002	
	AE13	-						AUG 1	2 2002	
	AF13							Fechnology	Center 2	00
	AG13								7.7.114	
	AH13	 		 -						<u> </u>
	Al13				FORFION	LDAT			l	L
EXAMINER		-			FUREIGN	PAIL	ENT DOCUMENTS			
NITIAL		DOC	UMENT NUM	BER	DATE		COUNTRY	CLASS	SUB- CLASS	TRANSLATION
	AJ13				_		RECEIVE	: D		
	AK13						AUG 1 5 20	02		
	AL13						Technology Cente	r 2100		
	AM13									
			ОТНІ	ER (inc	cluding Aut	hor, Ti	tle, Date, Pertinent Pages,	etc.)		
AB	AN	<u>13</u>					ion of a System for Reagent Socie			
AB	AO	<u>13</u>	Leach, Andre Science Ltd.,	w R. a Augus	ınd Hann, M st 2000, Vol.	ichael 5, No.	M., "The <i>in silico</i> world of virt 8, pp. 326-336.	ual libraries," <i>E</i>	rug discover	<i>y today</i> , Elsevier
			Loland, Burte	л А. <i>ө</i>	t al.: "Manac	ina the	Combinatorial Explosion," J	Chom. Inf. Go	mput Soi. A	merioon
	AP	<u>13</u>	Chemical So	ciety, 1	1997, Vol. 37	, Ňo. ¹	I, pp. 62-70.		,	
M	, , AQ	<u>13</u>	Lobanov, Vic Libraries," <i>J.</i> 470.	tor S. a Chem.	and Agrafioti Inf. Compu	is, Dim <i>t. Sci.</i> ,	itris K., "Stochastic Similarity American Chemical Society,	Selections from March/April 20	m Large Com 00, Vol. 40, N	binatorial No. 2, pp. 460-
	AR	<u>13</u>	Matter, Hans Diverse Com 1211-1225.	and P pound	ötter, Thorst Subsets," <i>J</i>	en, "C . <i>Chen</i>	omparing 3D Pharmacophore n. Inf. Comput. Sci., American	Triplets and 2 Chemical Soc	D Fingerprint iety, 1999, Vo	s for Selecting ol. 39, No. 6, pp.
EXAMINER		mel	Kada	 				DATE CONS	IDERED	

ATTY. DOCKET NO. 1503.0200006 FORM PTO-1449 APPLICANT AUG 1 4 2002 Agrafiotis et al TION DISCLOSURE STATEMENT GROUR TECH OCHICH 1600/2900 FILING DATE March 12, 2001 **U.S. PATENT DOCUMENTS EXAMINER** INITIAL DATE NAME CLASS SUB-FILING DATE DOCUMENT **CLASS** NUMBER **AA14** AB14 AC14 AD14 AE14 AF14 AG14 AH14 AI14 FOREIGN PATENT DOCUMENTS **EXAMINER** COUNTRY DOCUMENT NUMBER CLASS TRANSLATION INITIAL DATE SUB-CLASS AJ14 No RECEIVED No AK14 AUG 1 5 2002 AL14 No Technology Center 2100 AM14 No OTHER (Including Author, Title, Date, Pertinent Pages, etc.) Matter, Hans, "Selecting Optimally Diverse Compounds from Structure Databases: A Validation Study of Two-ΆN 14 Dimensional and Three-Dimensional Molecular Descriptors," J. Med. Chem., American Chemical Society, 1997, Vol. 40, No. 8, pp. 1219-1229. i. Sadowski, Jens and Kubinyi, Hugo, "A Scoring Scheme for Discriminating between Drugs and Nondrugs," J. AO <u>14</u> Med. Chem., American Chemical Society, 1998, Vol. 41, No. 18, pp. 3325-3329. Schnur, Dora, "Design and Diversity Analysis of Large Combinatorial Libraries Using Cell-Based Methods," J. ΑP 14 Chem. Inf. Comput. Sci., American Chemical Society, 1999, Vol. 39, No. 1, pp. 36-45. Schuffenhauer, Ansgar et al., "Similarity Searching in Files of Three-Dimensional Chemical Structures: Analysis of the BIOSTER Database Using Two-Dimensional Fingerprints and Molecular Field Descriptors," J. Chem. Inf. AQ 14 Comput. Sci., American Chemical Society, 2000, Vol. 40, No. 2, pp. 295-307. Turner, David B. et al., "Rapid Quantification of Molecular Diversity for Selective Database Acquisition," J. AR <u>14</u> Chem. Inf. Sci., American Chemical Society, 1997, Vol. 37, No. 1, pp. 18-22. **EXAMINER**

EXAMINER: Initial if reference considered, whether or not citation is in conformance with MPEP 609. Draw line through citation if not in

conformance and not considered. Include copy of this form with next communication to Applicant.

ATTY. DOCKET NO. 1503.0200006

APPLICATION NO. 09/802,956

APPLICANT Agrafiotis et al.

	*ORMATIO	N DIS	CLOSURE STA	TEME	<u>1T</u>	FII	rafiotis et al. LING DATE rch 12, 2001	GROUP 2123		
					U.S. P		DOCUMENTS			
XAMINER NITIAL			CUMENT MBER	DAT	E	NAM		CLASS	SUB- CLASS	FILING DATE
	AA15	↓		ļ				<u> </u>		
	AB15	-				-	P	ECEI	VFD-	
	AC15	+		 ,						
	AD15	+-			- -			AUG 1 2	2002	
	AE15	╂				-	Tabl		. 0.100	
	AF15						recr	hology Co	Inter 2100	
	AG15	+-		1						
	AH15 Al15	+				1				
	Allo	1		<u> </u>	FORFIGI	N PATE	NT DOCUMENTS			
XAMINER	4				TONLIGI	I	INT DOCUMENTS			
NITIAL	i di C	DOG	CUMENT NUM	BER	DATE		COUNTRY	CLASS	SUB- CLASS	TRANSLATIO
	AJ15						RECEIN	/ED		
	AK15						AUG 1 5	2002		N
	AL15						Technology Ce	rter 2100		٨
	AM15		<u> </u>							١
			OTU	ED //=	aludina Au	hor Ti	tle, Date, Pertinent Pages, e	. <u> </u>		
	AO	<u>15</u>	November/D	ecemb	er 1999, Vo	I. 1, No	punds," <i>J. Comb. Chem.</i> , Ame . 6, pp. 524-533. Diversity of Combinatorial Lit <i>211th ACS National Meetin</i>	praries by an I	Encoding of M	lolecular Surfac D-CINF.
	AP	<u>15</u>					nd visualization of molecular of Publishers B.V., 1996, Vol. 2,		nbinatorial lib	raries,"
			Ì							11 (1001)
	AQ	<u>15</u>	Bellman, R.E	., Ada	ptive Contro	ol Proce	sses: A Guided Tour, Princeto	on Univ. Press	s, Princeton, I	NJ (1961).
	AQ	<u>15</u>				-	sses: A Guided Tour, Princeto			

Page 16 of 36 APPLICATION NO. ATTY. DOCKET NO. 1503.0200006 09/802,956 FORM PTO-1449 APPLICANT Agrafiotis et al. ION DISCLOSURE STATEMENT GROUP FILING DATE March 12, 2001 2123 **U.S. PATENT DOCUMENTS EXAMINER CLASS** FILING DATE DOCUMENT DATE NAME SUB-INITIAL **CLASS** NUMBER AA16 AB16 AC16 AD16 AE16 Technology Center 2100 AF16 **AG16** AH16 Al16 FOREIGN PATENT DOCUMENTS **EXAMINER** DOCUMENT NUMBER COUNTRY **CLASS** TRANSLATION INITIAL DATE SUB-CLASS RECEIVED AJ16 No AUG 1 5 2002 No AK16 No AL16 Technology Center 2100 AM16 No OTHER (Including Author, Title, Date, Pertinent Pages, etc.) Johnson, M.A., and Maggiora, G.M., Concepts and Applications of Molecular Similarity, John Wiley and Sons, ΑN 16 New York, NY (1990). ΑO Kohonen, T., Self-Organizing Maps, Springer-Verlag, Heidelberg, Germany (1995). 16 ΑP <u>16</u> Oja, E., Subspace Methods of Pattern Recognition, Research Studies Press, Letchworth, England (1983). Agrafiotis, D.K., "A New Method For Analyzing Protein Sequence Relationships Based On Sammon Maps," AQ <u>16</u> Protein Science, Cambridge University Press, Vol. 6, No. 2, February 1997, pp. 287-293.

EXAMINER Samuel Kroda

16

AR

DATE CONSIDERED

EXAMINER: Initial if reference considered, whether or not citation is in conformance with MPEP 609. Draw line through citation if not in conformance and not considered. Include copy of this form with next communication to Applicant.

Copy of International Search Report issued October 18, 1999, for Appl. No. PCT/US99/09963, 7 pages.

AUG 0 9 ZOUZ

FORM PTO-1449

ATTY. DOCKET NO. 1503.0200006	APPLICATION NO. 09/802,956
APPLICANT	

ATION DISCLOSURE STATEMENT GROUP FILING DATE March 12, 2001 2123 **U.S. PATENT DOCUMENTS EXAMINER** NAME **CLASS** FILING DATE DOCUMENT DATE SUB-INITIAL NUMBER **CLASS AA17** AB17 AC17 AD17 AUG 1 AE17 AF17 Technology Center 2100 **AG17** AH17 Al17 **FOREIGN PATENT DOCUMENTS EXAMINER** DOCUMENT NUMBER COUNTRY CLASS TRANSLATION INITIAL DATE SUB-CLASS RECEIVED AJ17 No AK17 No AUG 1 5 2002 Νo AL17 Technology Center 2100 **AM17** No OTHER (Including Author, Title, Date, Pertinent Pages, etc.) Amzel, L.M., "Structure-based drug design," Current Opinion in Biotechnology, Vol. 9, No. 4, August 1998, pp. AN 17 366-369. Blaney, J.M. and Martin, E.J., "Computational approaches for combinatorial library design and molecular AO diversity analysis," Current Opinion in Chemical Biology, Current Biology Ltd., Vol. 1, No. 1, June 1997, pp. 54-<u>17</u> 59. Brown, R.D. and Clark, D.E., "Genetic diversity: applications of evolutionary algorithms to combinatorial library design," *Expert Opinion on Therapeutic Patents*, Vol. 8, No. 11, November 1998, pp. 1447-1459. ΑP 17 Caflisch, A. and Karplus, M., "Computational combinatorial chemistry for de novo ligand design: Review and assessment," Perspectives in Drug Discovery and Design, ESCOM Science Publishers B.V., Vol. 3, 1995, pp. AQ <u>17</u> 51-84. Danheiser, S.L., "Current Trends in Synthetic Peptide and Chemical Diversity Library Design," Genetic AR 17 Engineering News, May 1, 1994, pp. 10 and 31. **EXAMINER**

APPLICATION NO. ATTY. DOCKET NO. 1503.0200006 AUG 1 4 700 FORM PTO-1449 APPLICANT Agrafiotis et al. ON DISCLOSURE STATEMENT TECH CENTER 1800/\$901 FILING DATE GROUP 2123 March 12, 2001 **U.S. PATENT DOCUMENTS EXAMINER** DATE NAME **CLASS** SUB-FILING DATE INITIAL DOCUMENT NUMBER CLASS **AA18 AB18** AC18 AD18 2002 AUG 1 AE18 AF18 Tednnology Center 2100 **AG18** AH18 **AI18** FOREIGN PATENT DOCUMENTS **EXAMINER** DOCUMENT NUMBER COUNTRY **CLASS** SUB-TRANSLATION INITIAL DATE **CLASS** AJ18 Yes No Yes AK18 No Yes AL18 No Technology Center 2100 **AM18** Yes No OTHER (Including Author, Title, Date, Pertinent Pages, etc.) Eichler, U. et al., "Addressing the problem of molecular diversity," Drugs of the Future, Prous Science, Vol. 24, ΑN <u>18</u> No. 2, 1999, pp. 177-190. Felder, E.R. and Poppinger, D., "Combinatorial Compound Libraries for Enhanced Drug Discovery Approaches," AO 18 Advances in Drug Research, Academic Press, Vol. 30, 1997, pp. 112-199. Geysen, H.M. and Mason, T.J., "Screening Chemically Synthesized Peptide Libraries for Biologically-Relevant ΑP <u>18</u> Molecules, "Biorganic & Medicinal Chemistry Letters, Pergamon Press Ltd., Vol. 3, No. 3, 1993, pp. 397-404. Gobbi, A. et al., "New Leads By Selective Screening of Compounds From Large Databases," Abstracts of AQ <u>18</u> Papers Part 1: 213th ACS National Meeting, April 13-17, 1997, p. 67-CINF. Houghten, R.A. et al., "The Use of Synthetic Peptide Combinatorial Libraries for the Identification of Bioactive AR <u>18</u> Peptides," Peptide Research, Vol. 5, No. 6, 1992, pp. 351-358. **EXAMINER** EXAMINER: Initial if reference considered, whether or not citation is in conformance with MPEP 609. Draw line through citation if not in conformance and not considered. Include copy of this form with next communication to Applicant.

	Page 19 of 36
	APPLICATION NO. 09/802,956
APPLICANT Agrafiotis et al.	

1 Am	\$/		TO-1449			PPLICANT grafiotis et al.			
Ameria 18	OKMATION	1 DISC	CLOSURE STATEM	ENT	F	ILING DATE arch 12, 2001	GROUP 2123		
				U		NT DOCUMENTS	12123		
EXAMINER INITIAL		DOC NUM		NTE .	NAI	ME	CLASS	SUB- CLASS	FILING DATE
	AA19	1							
	AB19							1	
	AC19	 	· <u></u>				HECE	EIVE)
	AD19				-		AUC 1	9 2002	-
	AE19	 			_		AUG I	2 2002	
	AF19				1	To Table	chnology	Center 2	100
	AG19 AH19	1					3,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,	OUTION E	
	Al19	1-		,, , , , , , , , , , , , , , , , , , ,					
1	7410	<u> </u>		FOR	EIGN PAT	TENT DOCUMENTS	1	<u> </u>	-
EXAMINER INITIAL		DOC	UMENT NUMBER			COUNTRY	CLASS	SUB- CLASS	TRANSLATION
	AJ19					RECEIVED			Yes No
	AK19					AUG 1 5 2002			Yes No
	AL19					Technology Center 21	00		Yes No
	AM19					160thology contol E			Yes
							<u> </u>		No
MS	AN	<u>19</u>	Klopman, G., "Ar	tificial Inte	elligence A	Title, Date, Pertinent Pages, et approach to Structure-Activity Sturganic Molecules," <i>J. Am. Chem.</i> . 7315-7321.	ıdies. Comp	uter Automat can Chemica	ed Structure I Society, Vol.
	AO	<u>19</u>	Lajiness, M.S. et Quantitative Stru	<i>al</i> ., "Imple cture-Acti	ementing I ivity Relati	Drug Screening Programs Using onships in Drug Design, Alan R.	Molecular Si Liss, Inc., 19	milarity Meth 189, pp. 173-1	ods," <i>QSAR:</i> 176.
	АР	<u>19</u>	Loew, G.H. <i>et al.</i> Publishing Corpo	, "Strategi ration, Vo	ies for Indi ol. 10, No.	rect Computer-Aided Drug Desiç 4, 1993, pp. 475-486.	gn," <i>Pharmac</i>	eutical Rese	<i>arch</i> , Plenum
	AQ	<u>19</u>	Lynch, M.F. et al Society, Vol. 25,			e Storage and Retrieval," <i>J. Chei</i> , pp. 264-270.	m. Inf. Compl	ut. Sci., Amer	rican Chemical
	AR	<u>19</u>	Myers, P.L. <i>et al.</i> 6, No. 7, July/Au	, "Rapid, I gust 1997	Reliable D	rug Discovery," <i>Today's Chemis</i> 3, 51 & 53.	t At Work, An	nerican Chen	nical Society, Vol.
EXAMINER	Aan	nel	Brida				DATE CONS	DEBED	

	Page 20 of 36
ATTY. DOCKET NO. 1503.0200006	APPLICATION NO. 09/802,956
APPLICANT Agrafiotis et al.	

TRATE TRAIN	OTTAMA	N DISCL	OSURE STA	TEMEN	IT	Ag	rafiotis	et al	·				
TRA							LING DAT				GROUP 2123		
			 		U.S. P.		L DOCUM						
EXAMINER INITIAL		DOCU NUMB		DATE	=	NAM	E			(CLASS	SUB- CLASS	FILING DATE
	AA20												
	AB20												
	AC20										EC	EIVE	
	AD20											-1 V L_ L	!
	AE20	<u> </u>									AUG 1	2 2002	
	AF20									-			
	AG20									Ido	hnology	Center 2	100
	AH20			ļ		ļ							
	Al20	Į.											
					FOREIGN	1 PATI	ENT DOC	JMENTS					
EXAMINER INITIAL		DOCU	MENT NUM	BER	DATE		COUNTR	RE RE	CEI	VE.	CLASS D	SUB- CLASS	TRANSLATION
	AJ20												Yes
	11/00	 						AU	<u>G 15</u>	<u> 240</u>	17		No
	AK20	1							-la C		- 0100		Yes No
	AL20							Techn	ology C	ente	r 2100		Yes No
	AM20												Yes No
	1	-L	OTH	FR (Inc	cluding Aut	hor T	itle Date	Pertinen	t Pages	etc))		
AB	AN	20	Pabo, C.O. a American Ch	nd Sud emical	chanek, E.G Society, Vo	., "Con I. 25, N	nputer-Aid No. 20, 198	ed Model 36, pp. 59	-Building 187-599	g Stra	tegies for P	rotein Desig	n," <i>Biochemistry</i> ,
	AO	<u>20</u>	Saudek, V. e lournal of Pe	t al., "S eptide l	Solution Con Protein Res.	format , Munk	ion of End sgaard Int	othelin-1 ernationa	by H NN I Publisi	MR, Cl hers L	D, and Mole td., Vol. 37	ecular Mode , No. 3, 199	ling," <i>International</i> I, pp. 174-179.
	АР	<u>20</u> (1		ation a	and Lead Op	otimiza							al Approach to ol. 118, No. 5,
	AQ		/an Drie, J.H .td., Vol. 3, N					to virtual	library d	lesign	," Drug Dise	covery today	, Elsevier Science
1	AR		Walters, W.F I, April 1998			reeninç	g - an over	view," <i>Dr</i>	ug Disco	overy	today, Else	vier Science	Ltd., Vol. 3, No.
EXAMINER	An	mell	uda				•			DA	TE CONSI	DERED	
EXAMINER: In			nsidered. wh	nether	or not citatio	n is in	conformar	nce with I	MPEP 6	09. D	raw line thr	ough citation	if not in
conformance a													

	 	Page	21	or	36
ATTY. DOCKET NO. 1503.0200006	APPLICATION 09/802,956	NO.			
APPLICANT Agrafiotis et al.					
ETLING DAME	CDOUD				

3	MON F	ORM :	PTO-1449		_	AP	PLICANT rafiotis et al.		_,,,,,,	
3 THE THROP	ORMATIO	N DIS	CLOSURE ST	'ATEMEI	<u>NT</u>	FI	LING DATE	GROUP 2123		
					U.S. P		T DOCUMENTS			
EXAMINER INITIAL			CUMENT MBER	DAT	E	NAM	E	CLASS	SUB- CLASS	FILING DATE
	AA21									
···	AB21	<u> </u>				<u> </u>		BEAL	EIVE	
	AC21	+		+		 		ILUL	IVLL	<i>J</i>
	AD21 AE21	+					<u>-</u>	AUG 1	2 2002	
	AF21			+			····			
	AG21							chnology	Center 2	100
	AH21									
	Al21									
					FOREIGN	V PATI	ENT DOCUMENTS			
EXAMINER INITIAL		DOG	CUMENT NU	MBER	DATE		COUNTRY	CLASS	SUB- CLASS	TRANSLATION
	AJ21						RECEIVE	P		Yes No
	AK21			-			AUG 1 5 200	2		Yes No
	AL21						Technology Cente	2100		Yes No
	AM21									Yes No
	·		OTI	IER (In	cluding Auti	hor, T	itle, Date, Pertinent Pages, et	c.)	•	
AB	AN	<u>21</u>	Weber, L., Elsevier Sc	"Evolutio ience Lt	onary combir d., Vol. 3, No	natoria o. 8, A	I chemistry: application of gene ugust 1998, pp. 379-385.	tic algorithms	s," Drug Disc	overy today,
	AO	<u>21</u>	Weber, L. & Algorithm," 2280-2282.	et al., "O Angewa	optimization of andte Chemic	of the E	Biological Activity of Combinator national Edition in English, VCH	rial Compour I, Vol. 34, No	d Libraries b b. 20, Noveml	y a Genetic oer 3, 1995, pp.
	AP	<u>21</u>	Structure-B	ased Dr	rua Desian."	from N	ug Discovery Process by Integr Molecular Diversity and Combina American Chemical Society, 19	atorial Chem	stry: Librarie	Chemistry and s and Drug
	AQ	<u>21</u>	Saund, E., and Machir	"Dimens e Intelli	sionality-Red gence, IEEE	luction , Vol. 1	Using Connectionist Networks, I1, No. 3, March 1989, pp. 304-	" IEEE Trans 314.	sactions on P	attern Analysis
			HODD and	da		-+" C'	omiato in Britain The Bound C	valore of Ob	minter V-1 0	0 No. 4
EXAMINER	AR	<u>21</u>	"3DP gains 1996, p. 22		searcn pater	it", Ch	emistry in Britain, The Royal Sc	DATE, CONS		∠, No. 1, January

INFORMATION DISCLOSURE STATEMENT

ATTY. DOCKET NO. 1503.0200006

APPLICATION 09/802,9

APPLICANT

Agrafiotis et al.

AUG 1 4 7002

00

		4 DIS	CLOSURE STA	TEME	<u>N'1'</u>	Agrariotis et al.				6 1 2 /00/
TO TRANS		•				FILING DATE March 12, 2001		GROUP 2123	TEOU(
		***			U.S. P	ATENT DOCUMENTS			IFOU OF	
EXAMINER INITIAL			CUMENT MBER	DAT	E	NAME	CI	_ASS	SUB- CLASS	FILING DATE
	AA22	1								
	AB22						RF	CE	VED	
	AC22									
	AD22						F	UG 1	2 2002	
	AE22						_		<u> </u>	
	AF22	<u> </u>					regnn	ology (Center 210	0
	AG22	ļ		<u> </u>						
·	AH22			ļ						
	Al22	<u> </u>	<u>-</u> <u>-</u>			<u> </u>				
		T			FOREIGI	N PATENT DOCUMENTS			1	1
XAMINER NITIAL		DOG	CUMENT NUM	BER	DATE	COUNTRY	CI	_ASS	SUB- CLASS	TRANSLATIO
	AJ22)
	AK22					RECEIV	ED			Y
	AL22					AUG 1 5 2	002			. 1
,,	AM22				<u> </u>	Technology Cent	er 210	0		Y
· . · . · · · · · · · · · · · · · · · ·			OTH	5D //=	alisation Ass	thor, Title, Date, Pertinent Pages			<u>. </u>	
A S	AO	<u>22</u>				gorithms for Maximizing Molecula ican Chemical Society, Vol. 37, No				eal Information
)							
	АР	22	with regressi	on, <i>K</i> -	nearest neig	tion of pyrolysis mass spectra by f hbour, neural and decision-tree m , August 20, 1997, pp. 389-407.				
	AP	<u>22</u> <u>22</u>	with regressi Science B.V.	on, K- , Vol. and K	nearest neig 348, No. 1-3 	hbour, neural and decision-tree m	ethods"	, <i>Analytic</i>	ructure-Activi	cta, Elsevier ty Relationship
			with regressi Science B.V. Andrea, T.A. of Dihydrofol 9, 1991, pp.	and Kate Re 2824-2	nearest neig 348, No. 1-3 (alayeh, H., ' eductase Inh 2836.	hbour, neural and decision-tree many states and the control of the	n Quant nistry, A	itative Sti	ructure-Activi Chemical Sociationship Ana	eta, Elsevier ty Relationship ciety, Vol. 34, I

Page 23 of 36 ATTY. DOCKET NO. 1503.0200006 APPLICATION NO. 09/802,956 FORM PTO-1449 APPLICANT Agrafiotis et al. TION DISCLOSURE STATEMENT FILING DATE GROUP March 12, 2001 2123 **U.S. PATENT DOCUMENTS EXAMINER** DOCUMENT DATE NAME CLASS FILING DATE INITIAL SUB-NUMBER CLASS AA23 AB23 AC23 AD23 AE23 Technology Center 2100 AF23 AG23 AH23 A123 **FOREIGN PATENT DOCUMENTS EXAMINER** COUNTRY INITIAL DOCUMENT NUMBER DATE CLASS SUB-TRANSLATION CLASS RECEIVED AJ23 Yes No AUG 1 5 2002 Yes AK23 No Technology Center 2100 AL23 Yes No **AM23** Yes No OTHER (Including Author, Title, Date, Pertinent Pages, etc.) Aoyama, T. and Ichikawa, H., "Obtaining the Correlation Indices between Drug Activity and Structural ΑN 23 Parameters Using a Neural Network", Chemical & Pharmaceutical Bulletin, Pharmaceutical Society of Japan, Vol. 39, No. 2, February 1991, pp. 372-378. AO <u>23</u> "ArQule Inc", from http://www.bioportfolio.com/arqule/products.htm, 5 pages, (March 18, 1998). Baum, R.M., "Combinatorial Approaches Provide Fresh Leads for Medicinal Chemistry", Chemical & ΑP <u>23</u> Engineering News, American Chemical Society, February 7, 1994, pp. 20-26. Bentley, J. L., "Multidimensional Binary Search Trees Used for Associative Searching", Communications of the AQ 23 ACM, Association for Computing Machinery, Inc., Vol. 18, No. 9, September 1975, pp. 509-517. Bottou, L. and Vladimir Vapnik, "Local Learning Algorithms", Neural Computation, Massachusetts Institute of AR 23 Technology, Vol. 4, No. 6, pp. 888-900, (November 1992).

EXAMINER Samuelly sola

DATE CONSIDERED 12/03/03

Page 24 of 36 ATTY. DOCKET NO. APPLICATION NO. 1503.0200006 09/802,956 FORM PTO-1449 APPLICANT Agrafiotis et al. FION DISCLOSURE STATEMENT FILING DATE GROUP March 12, 2001 2123 **U.S. PATENT DOCUMENTS EXAMINER** DOCUMENT DATE NAME **CLASS** SUB-FILING DATE INITIAL NUMBER **CLASS** AA24 AB24 AC24 AD24 AE24 Technology Center 2100 AF24 AG24 AH24 AI24 **FOREIGN PATENT DOCUMENTS EXAMINER** COUNTRY **CLASS** TRANSLATION INITIAL DOCUMENT NUMBER DATE SUB-CLASS RECEIVED AJ24 Yes No AK24 Yes AUG 1 5 2002 No Yes AL24 Technology Center 2100 No AM24 Yes No OTHER (Including Author, Title, Date, Pertinent Pages, etc.) Boulu, L.G. and Crippen, G.M., "Voronoi Binding Site Models: Calculation of Binding Modes and Influence of Drug Binding Data Accuracy", Journal of Computational Chemistry, John Wiley & Sons, Inc., Vol. 10, No. 5, July/August 1989, pp. 673-682. AN 24 Boulu, L.G. et al., "Voronoi Binding Site Model of a Polycyclic Aromatic Hydrocarbon Binding Protein", Journal of AO <u>24</u> Medicinal Chemistry, American Chemical Society, Vol. 33, No. 2, 1990, pp. 771-775. Brown, R. D. and Martin, Y.C., "Use of Structure-Activity Data To Compare Structure-Based Clustering Methods and Descriptors for Use in Compound Selection", Journal of Chemical Information and Computer Sciences, Vol. 36, No. 3, 1996, pp. 572-584. Cacoullos, T., "Estimation of a Multivariate Density", Annals of The Institute of Statistical Mathematics, The AQ <u>24</u> Institute of Statistical Mathematics, Vol. 18, No. 2, 1966, pp. 179-189. Clark, R.D., "OptiSim: An Extended Dissimilarity Selection Method for Finding Diverse Representative Subsets", Journal of Chemical Information and Computer Sciences, American Chemical Society, Vol. 37, No. 6, 1997, pp. AR 24 1181-1188. **EXAMINER EXAMINER**: Initial if reference considered, whether or not citation is in conformance with MPEP 609. Draw line through citation if not in conformance and not considered. Include copy of this form with next communication to Applicant.

ATTY.	DOCKET	NO.
1503.	0200006	

APPLICATION NO.

AUG US 2005	.						TY. DOCKET NO. 03.0200006	09/80	CATION NO. 2,956	
%	F	ORM P	ro-1449				PLICANT			-
ALEMY & TRAINERS	ORMATION	1 DISC	LOSURE ST	ATEME	NT TN		rafiotis et al. LING DATE	GROUP		
						Ma	rch 12, 2001	2123		
		т			U.S. P	ATEN	T DOCUMENTS		Γ	
EXAMINER INITIAL		DOCI	UMENT BER	DAT	E	NAM	E	CLASS	SUB- CLASS	FILING DATE
	AA25									
	AB25						RI	ECEI'	VED	
	AC25			_						·
	AD25	ļ						AUG 1 2	2002	
	AE25	-		-			Took	0.0	0400	
	AF25		·				recn	nology Ce	nter 2100	
	AG25	-		4			-		(
	AH25	<u> </u>		-						
	A125		······································							
TVANAINICO	1				FOREIGN	PATE	ENT DOCUMENTS			
EXAMINER INITIAL		DOC	UMENT NUN	/BER	DATE		COUNTRY	CLASS	SUB- CLASS	TRANSLATION
	AJ25						RECE	VED		Ye: No
	AK25						AUG 1 5	2002		Yes No
	AL25		<u> </u>				Technology C	enter 2100)	Ye: No
	AM25									Ye: No
	<u>i</u>	ł	OTL	IED //-	mlerelimes Aret	bor T	I itle, Date, Pertinent Pages, et	<u> </u>	<u> </u>	INC
₩ —	AN	<u>25</u>					volutionary algorithms in compu SCOM Science Publishers B.V.			
	AO	<u>25</u>	Steroids to	Carrier	et al., "Compa Proteins", <i>Jo</i> 1988, pp. 59	urnal d	Molecular Field Analyisis (CoM of The American Chemical Soci 67.	FA). 1. Effectety, America	t of Shape or n Chemical S	Binding of ociety, Vol. 110,
	АР	<u>25</u>					Analysis. A Novel Approach to lay 1974, pp. 533-535.	the Problem	of Drug Desi	ign", <i>Journal of</i>
	AQ	<u>25</u>	Crippen, G. Vol. 8, No. 7	M., "Vo 7, Octol	oronoi Bindin ber/Novembe	g Site l er 1987	Models", <i>Journal of Computatic</i> 7, pp. 943-955.	nal Chemisti	ry, John Wiley	/ & Sons, Inc.,
	AR	<u>25</u>		s on M			or Finding Best Matches in Logare, Association for Computing N			
A #										

Page 26 of 36 ATTY. DOCKET NO. APPLICATION NO. 1503.0200006 09/802,956 FORM PTO-1449 APPLICANT Agrafiotis et al. ION DISCLOSURE STATEMENT FILING DATE GROUP March 12, 2001 2123 **U.S. PATENT DOCUMENTS EXAMINER** FILING DATE DOCUMENT DATE NAME **CLASS** SUB-INITIAL NUMBER CLASS AA26 AB26 AC26 AD26 AE26 AF26 Technology Center 2100 AG26 AH26 A126 **FOREIGN PATENT DOCUMENTS EXAMINER** COUNTRY CLASS INITIAL DOCUMENT NUMBER DATE SUB-TRANSLATION CLASS RECEIVED AJ26 Yes No AUG 1 5 2002 AK26 Yes No AL26 Yes Technology Certer 2100 No AM26 Yes No OTHER (Including Author, Title, Date, Pertinent Pages, etc.) Friedman, J.H., "Fitting Functions To Noisy Data In High Dimensions", Department of Statistics- Stanford AN 26 University Technical Report No. 101, (August, 1988). Gallop, M. A. et al., "Applications of Combinatorial Technologies to Drug Discovery. 1. Background and Peptide AO <u>26</u> Combinatorial Libraries", Journal of Medicinal Chemistry, American Chemical Society, Vol. 37, No. 9, April 29, 1994, pp. 1233-1251. Ghose, A. K. and Crippen, G.M., "Use of Physicochemical Parameters in Distance Geometry and Related Three-Dimensional Qantitative Structure-Activity Relationships: A Demonstration Using Escherichia coli AΡ 26 Dihydrofolate Reductase Inhibitors", Journal of Medicinal Chemistry, American Chemical Society, Vol. 28, No. 3, 1985, pp. 333-346. Good, A. C. et al., "Structure-Activity Relationships from Molecular Similarity Matrices", Journal of Medicinal AQ 26 Chemistry, American Chemical Society, Vol. 36, No. 4, February 19, 1993, pp. 433-438. Gordon, E. M. et al., "Applications of Combinatorial Technologies to Drug Discovery. 2. Combinatorial Organic AR Synthesis, Library Screening Strategies, and Future Directions", Journal of Medicinal Chemistry, American <u>26</u> Chemical Society, Vol. 37, No. 10, May 13, 1994, pp. 1385-1401.

EXAMINER: Initial if reference considered, whether or not citation is in conformance with MPEP 609. Draw line through citation if not in conformance and not considered. Include copy of this form with next communication to Applicant.

EXAMINER

Page 27 of 36

AUG O 9 200	Š						03.0200006	09/80	2,956	
4 3	3 /		PTO-1449				PLICANT rafiotis et al.			
ANTA TRANSPORT	MMTION	1 DIS	CLOSURE STA	TEMEN	<u>VT</u>	FI	LING DATE	GROUP 2123		
					U.S. P.	ATEN	T DOCUMENTS			
EXAMINER INITIAL			CUMENT MBER	DATI	E	NAM	E	CLASS	SUB- CLASS	FILING DATE
	AA27									
	AB27								EIVEI	
	AC27	<u> </u>							-IVE)
	AD27							AUG 1	2 2002	
	AE27	ļ								
	AF27							chnology	Center 2	100
	AG27									00
	AH27									
	Al27	<u> </u>								
		T			FOREIGN	PATE	NT DOCUMENTS	-		
EXAMINER INITIAL		DOC	CUMENT NUM	BER	DATE		COUNTRY	CLASS	SUB- CLASS	TRANSLATION
	AJ27						RECEIVE	D		Yes No
	AK27						AUG 1 5 20	02		Yes No
	AL27						Technology Cent			Yes No
-	AM27						(eciliology cent	7 2 100		Yes
			ОТН	FR (In	cluding Aut	hor Ti	tle, Date, Pertinent Pages, etc	.)	<u> </u>	No
AB	AN	<u>27</u>		4., "Re	presentation	of Sin	nilarity Matrices By Trees", Journ		nerican Statis	stical Association,
	AO	<u>27</u>	Hopfinger, A Molecular Sh No. 24, Nove	ape A	nalysis", <i>Jou</i>	ırnal ol	on of Dihydrofolate Reductase In the American Chemical Society 7206.	hibition by B , American (Baker Triazine Chemical Soc	es Based upon ciety, Vol. 102,
	AP	27	Jackson, R. Biology Ltd.,	C., "Up Vol. 6,	odate on com , No. 6, Dece	nputer- ember	aided drug design", <i>Current Opi</i> 1995, pp. 646-651.	nion in BIO1	FECHNOLOG	GY, Current
	AQ	<u>27</u>					eld analysis (CoMFA)", <i>Molecula</i> al, 1995, Ch. 12, pp. 291-331.	r Similarity i	n Drug Desig	<i>n</i> , ed. P. M.
1	AR	<u>27</u>	Kohonen, T., Springer-Ver				on of Topologically Correct Feat pp. 59-69.	ure Maps", <i>l</i>	Biological Cy	bernetics,
EXAMINER	Sam	nels	Brode				D	ATE CONS	1968 ED	
EXAMINER: In	itial if refe	rence	considered wh	nether	or not citatio	n is in	conformance with MPEP 609. I	Draw line thr	ough citation	if not in

conformance and not considered. Include copy of this form with next communication to Applicant.

Page 28 of 36 ATTY. DOCKET NO. APPLICATION NO. 1503.0200006 09/802,956 FORM PTO-1449 APPLICANT Agrafiotis et al. TION DISCLOSURE STATEMENT FILING DATE GROUP March 12, 2001 2123 **U.S. PATENT DOCUMENTS EXAMINER** DOCUMENT DATE NAME **CLASS** SUB-FILING DATE INITIAL NUMBER CLASS AA28 AB28 AC28 AD28 AUGI 1 200 AE28 AF28 rechnology Center 2100 AG28 AH28 AI28 **FOREIGN PATENT DOCUMENTS EXAMINER** COUNTRY INITIAL DOCUMENT NUMBER DATE CLASS SUB-TRANSLATION CLASS AJ28 Yes RECEIVED No AK28 Yes AUG 1 5 2002 No AL28 Yes No Technology Center 2100 AM28 Yes No OTHER (Including Author, Title, Date, Pertinent Pages, etc.) Koile, K. and Shapiro, R., "Building A Collaborative Drug Design System", Proceedings of the 25h Hawaii ΑN 28 International Conference on System Sciences, IEEE, 1992, pp. 706-716. Kowalski, B. R. and Bender, C. F., "Pattern Recognition. II. Linear and Nonlinear Methods for Displaying AO Chemical Data", Journal of the American Chemical Society, American Chemical Society, Vol. 95, No. 3, 28 February 7, 1973, pp. 686-693. Kruskal, J. B., "Nonmetric Multidimensional Scaling: A Numerical Method", Psychometrika, Vol. 29, No. 2, June, AΡ <u> 28</u> 1964, pp. 115-129. Lengauer, T. and Rarey, M., "Computational methods for biomolecular docking", Current Opinion in Structural AQ <u> 28</u> Biology, Current Biology Ltd, Vol. 6, No. 3, June, 1996, pp. 402-406. Luke, B. T., "Evolutionary Programming Applied to the Development of Quantitative Structure-Activity Relationships and Quantitative Structure-Property Relationships", *Journal of Chemical Information and Computer Sciences*, American Chemical Society, Vol. 34, No. 6, November/December 1994, pp. 1279-1287. AR <u>28</u>

EXAMINER: Initial if reference considered, whether or not citation is in conformance with MPEP 609. Draw line through citation if not in conformance and not considered. Include copy of this form with next communication to Applicant.

EXAMINER



	Page 29 of 36
ATTY. DOCKET NO. 1503.0200006	APPLICATION NO. 09/802,956
APPLICANT Agrafiotis et al.	
ETITMO DAME	CROTTR

100 - was	O MATTO	ם חדם	CLOSURE STATE	MEN	Ф	Ag	rafiotis et al.			
THE THE PARTY	ENTATIO	1 013	CLOSORE STATE	CILIIV	_		LING DATE rch 12, 2001	GROUP 2123		
					U.S. P		T DOCUMENTS			
EXAMINER INITIAL			CUMENT D.	ATE		NAM	E	CLASS	SUB- CLASS	FILING DATE
	AA29									
	AB29							DEC	EIVE	
	AC29							111	1 CIVE	<u>י</u>
	AD29	<u> </u>				<u> </u>		AHG	1 2 2002	
	AE29					<u> </u>				
	AF29							Technolo	gy Conter	2100
	AG29								0,	
	AH29	-						<u></u>		
	Al29					<u> </u>				
		40			FOREIG	N PATI	ENT DOCUMENTS	1		
EXAMINER INITIAL		DO	CUMENT NUMBE	R	DATE		COUNTRY	CLASS	SUB- CLASS	TRANSLATION
	AJ29						RECEI	VED		Yes No
	AK29						AUG 1 5	2002		Yes No
	AL29						Technology C	enter 2100)	Yes No
	AM29									Yes No
			OTUER	(100	Judina Aut	hor T	l itle, Date, Pertinent Pages, etc	2.)	<u> </u>	1 100
Mo	AN	<u>29</u>					al Chemistry Obviate Computer thers, Inc., Vol. 10, 1997, pp. 75		Design?", Re	eviews in
	AO	<u>29</u>	Martin, E. J. et a	al., " cina	Measuring I Chemistry	Diversi , Amer	ty: Experimental Design of Comican Chemical Society, Vol. 38,	nbinatorial Lil No. 9, April :	braries for Dro 28, 1995, pp.	ug Discovery", 1431-1436.
	AP	<u>29</u>	McMartin, C. an Journal of Comp 344.	d Be	ohacek, R.S <i>r-Aided Mo</i> i	S., "QX lecular	P: Powerful, rapid computer alg <i>Design</i> , Kluwer Academic Publ	orithms for s ishers, Vol. 1	structure-base I 1, No. 4, July	ed drug design", y 1997, pp. 333-
	AQ	<u>29</u>	Mezey, P. G. an No. 4, April 199	nd W 7, pj	/alker, P.D. p. 132-137.	, "Fuzz	y molecular fragments in drug r	esearch", <i>Di</i>	rug Discovery	rtoday, Vol. 2,
	AR	<u>29</u>	Müller, K., "On t Elsevier Science	he p	oaradigm sh V., Vol. 398	nift fron 3-399, \$	n rational to random design", <i>Jo</i> Special Issue, 1997, pp. 467-47	ournal of Mole 1.	ecular Structu	ure (Theochem),
EXAMINER	Jan	~ne	Warda			· · · ·	1	DATE CONS	IDERED	

Page 30 of 36 ATTY. DOCKET NO. APPLICATION NO. 1503.0200006 09/802,956 FORM PTO-1449 APPLICANT Agrafiotis et al. TION DISCLOSURE STATEMENT FILING DATE GROUP March 12, 2001 **U.S. PATENT DOCUMENTS EXAMINER** DATE CLASS FILING DATE INITIAL DOCUMENT NAME SUB-NUMBER CLASS **AA30 AB30** AC30 AD30 AE30 AF30 Technology Center 2100 AG30 **AH30** A130 **FOREIGN PATENT DOCUMENTS EXAMINER** INITIAL DOCUMENT NUMBER DATE COUNTRY CLASS SUB-TRANSLATION CLASS AJ30 Yes No Yes AK30 No Technology Center 2100 AL30 Yes No **AM30** Yes No OTHER (Including Author, Title, Date, Pertinent Pages, etc.) ΑN 30 Myers, P., "The Design Of A Universal, Informer[™] Library", COMBICHEM, INC., 10 Pages, Date unknown. Oinuma, H. et al., "Neural Networks Applied to Structure-Activity Relationships", Journal of Medicinal Chemistry, AO <u>30</u> Vol. 33, No. 3, pp. 905-908, (1990). Omohundro, S. M., "Bumptrees for Efficient Function, Constraint, and Classification Learning", Advances in AP 30 Neural Information Processing Systems 3, Morgan Kaufmann, 1991, 7 pages, unknown. Parrill, A. L., "Evolutionary and genetic methods in drug design", Drug Discovery today, Elsevier Science Ltd., AQ 30 Vol. 1, No. 12, December 1996, pp. 514-521. Polanski, J., "A neural network for the simulation of biological systems", Journal of Molecular Structure AR <u>30</u> (Theochem), Elsevier Science Ltd., Vol. 398-399, Special Issue, 1997, pp. 565-571. **EXAMINER**

EXAMINER: Initial if reference considered, whether or not citation is in conformance with MPEP 609. Draw line through citation if not in

conformance and not considered. Include copy of this form with next communication to Applicant.

::ODMA\MHODMA\SKGF_DC1;34595;2

AUG 0 9 200	2					ATTY. DOCKET 1503.0200006	NO.	APPLI 09/80	CATION NO 2,956	
	36/		PTO-1449			APPLICANT Agrafiotis et	al			
TATE TRAIN	ORMATIO	N DIS	SCLOSURE STA	TEME	<u>NT</u>	FILING DATE		GROUP		
		-			II S D	March 12, 200 ATENT DOCUMENT	,	2123	No.	
EXAMINER NITIAL			CUMENT MBER	DAT		NAME		CLASS	SUB- CLASS	FILING DATE
	AA31	1							CEACO	
	AB31									
	AC31	<u> </u>	·····				KE	CEIV	ED	
	AD31	4						UG 1 2 20	n2	ļ
	AE31									
	AF31						Techn	ology Cen	ter 2100	
	AG31 AH31							37		
	Al31	+								
	Aloi			<u> </u>	FOREIGN	PATENT DOCUME	NTS			<u> </u>
EXAMINER NITIAL		DO	CUMENT NUM	BER	DATE	COUNTRY	2 - 2 - 1 - 12 - 10 - 10 - 10 - 10 - 10	CLASS	SUB- CLASS	TRANSLATION
···	AJ31						DEOF	W. (5.5)		Yes
	AK31						RECE			No Yes
	AL31	-					AUG 1	5 2002		No Yes
		<u> </u>					Technology	L Center 210		No
	AM31	ŀ								Yes No
			ОТНІ	ER (In	cluding Autl	nor, Title, Date, Perl	tinent Pages, et	c.)		
AB	. AN	<u>31</u>	and cinnamic fuzzy system pp. 168-176.	acids s", <i>Jou</i>	on Listeria r urnal of Appli	nparison of quantitat nonocytogenes using ed Microbiology, Soc	g multiple linear r ciety for Applied b	egression, ar Bacteriology,	tificial neural Vol. 82, No.	network and 2, February 1997
	AO	<u>31</u>	Activity Relat	ionshi	ps and Quan	"Application of Gene titative Structure-Pro Chemical Society, Vo	perty Relationshi	ps", Journal	of Chemical	Information and
	AP	<u>31</u>	Sammon, Jr. IEEE, Vol. C-	, J. W. 18, No	., "A Nonlinea o. 5, May 196	ar Mapping for Data S 9, pp. 401-409.	Structure Analysi	s", <i>IEEE Trar</i>	nsactions on	Computers,
	AQ	<u>31</u>	Simon, Z. et (Steric) Differ 485-495.	al., "M ences	apping of Dit ", <i>Journal of</i>	nydrofolate-reductase Theoretical Biology,	e Receptor Site b Academic Press	y Correlation , Inc., Vol. 66	with Minima , No. 3, June	ll Topological 57, 1997, pp.
						Donostor Monsins by	Site-Directed Di	stances: A N	oval Mathad	
	AR	<u>31</u>	Pharmacolog	ical Le	eads", <i>Journa</i>	al of Chemical Informations 19 31, No.3, August 19	ation and Compu	ıter Sciences	,	of Predicting New
EXAMINER	AR	31	Pharmacolog	ical Le	eads", <i>Journa</i>	al of Chemical Inform	ation and Compu 991, pp. 386-392	ıter Sciences	•	of Predicting Nev

ATTY. DOCKET NO. 1503.0200006

APPLICATION NO. 09/802,956

APPLICANT

			····				rch 12, 2001	2123		
	 				U.S.	PATEN	T DOCUMENTS	1		
XAMINER NITIAL			CUMENT MBER	DATI	E	NAM	E	CLASS	SUB- CLASS	FILING DATE
· · · · · · · · · · · · · · · · · · ·	AA32	+						1		
	AB32	+					RF	CEIV	En	
	AC32	+					111			
	AD32	+						UG 1 2 2	bo2	
	AE32 AF32					-				
	AG32	+				+	- lechn	ology Cen	ter 2100	
	AH32	+								
	Al32	+								
		-			FOREIG	N PAT	ENT DOCUMENTS	<u> </u>		
XAMINER NITIAL		DOC	CUMENT NUME	BER	DATE		COUNTRY	CLASS	SUB- CLASS	TRANSLATIO
	AJ32						REC	EIVED		Ye
	AK32						AUG	1 5 2002		Ye
	AL32			· . ·			Technolog	y Center 21	90	Ye
	AM32	 								Ye
					1		ł			1
					-		itle, Date, Pertinent Pages, et Neural Network". IEEE Transa		ural Network	s, IEEE, Vol. 2,
AB	AN	<u>32</u>	Specht, D. F., No. 6, Novem	, "A G aber 1:	eneral Reg 991, pp. 56	ression 8-576.	itle, Date, Pertinent Pages, et Neural Network", IEEE Transadiction of the Solvatochromic Per Sciences, American Chemica	actions on Neu	ability Param	s, IEEE, Vol. 2, neter π ^H ₂ ", <i>Journ</i>
AB			Specht, D. F., No. 6, Novem Svozil, D. et a of Chemical II 342.	, "A G aber 19	eneral Reg 991, pp. 56 eural Netwe ation and C	ression 8-576. ork Prec	Neural Network", IEEE Transa diction of the Solvatochromic Pe er Sciences, American Chemica	octions on Neu olarity/Polariz al Society, Vol	ability Param . 37, No. 2, 1	s, IEEE, Vol. 2, neter π ^H ₂ ", <i>Journ</i> 1997, pp. 338-
AB			Specht, D. F., No. 6, Novem Svozil, D. et a of Chemical II 342.	, "A G ber 19	eneral Reg 991, pp. 56 eural Netwa ation and C	ression 8-576. ork Prec Compute	Neural Network", IEEE Transa	plarity/Polarizal Society, Vol	ability Param . 37, No. 2, 1	s, IEEE, Vol. 2, letter π^{H}_{2} ", Journ 1997, pp. 338-
AB	AO	<u>32</u>	Specht, D. F., No. 6, Novem Svozil, D. et a of Chemical II 342. Todorov, N. F ligand design pp. 175-192.	al., "Nonformal", Jou	eneral Reg 991, pp. 56 eural Netwo ation and C	ork Precompute M., "Evaluputer-A	Neural Network", IEEE Transaction of the Solvatochromic Por Sciences, American Chemical luation of a method for controllicated Molecular Design, ESCO	plarity/Polarizal Society, Vol	ability Param . 37, No. 2, 1 scaffold dive	s, IEEE, Vol. 2, neter π ^H ₂ ", <i>Journ</i> 1997, pp. 338- ersity in de novo ., Vol. 11, 1997,
AB .	AO	<u>32</u>	Specht, D. F., No. 6, Novem Svozil, D. et a of Chemical II 342. Todorov, N. Fligand design pp. 175-192. Torgerson, W Vol. 17, No. 4	al., "Nonformal", Jou	eneral Reg 991, pp. 56 eural Netwo ation and C Dean, P. N rnal of Con	ork Precompute A., "Evanputer-Ansional Section 2, pp. 46	Neural Network", IEEE Transaction of the Solvatochromic Por Sciences, American Chemical luation of a method for controllicated Molecular Design, ESCO	plarity/Polarizal Society, Vol	ability Param . 37, No. 2, 1 scaffold dive ablishers B.V	s, IEEE, Vol. 2, neter π ^H ₂ ", <i>Journ</i> 1997, pp. 338- ersity in de novo

Page 33 of 36 APPLICATION NO. ATTY. DOCKET NO. 1503.0200006 09/802,956 FORM PTO-1449 APPLICANT Agrafiotis et al. TION DISCLOSURE STATEMENT GROUP FILING DATE March 12, 2001 2123 **U.S. PATENT DOCUMENTS EXAMINER** DATE NAME CLASS SUB-FILING DATE INITIAL DOCUMENT CLASS NUMBER AA33 AB33 AC33 AD33 AE33 AF33 Technology Center 2100 AG33 **AH33** AI33 **FOREIGN PATENT DOCUMENTS EXAMINER** COUNTRY TRANSLATION DOCUMENT NUMBER CLASS SUB-INITIAL DATE CLASS AJ33 Yes No **AK33** Yes No Yes AL33 No Technology Center 2100 **AM33** Yes No OTHER (Including Author, Title, Date, Pertinent Pages, etc.) Vapnik, V. and Bottou, L., "Local Algorithms for Pattern Recognition and Dependencies Estimation", Neural AN 33 Computation, Massachusetts Institute of Technology, Vol. 5, No. 6, November 1993, pp. 893-909. Viswanadhan, V. N. et al., "Mapping the binding site of the nucleoside transporter protein: a 3D-QSAR study", AO 33 Biochimica et Biophysica Acta, Elsevier Science Publishers B.V., Vol. 1039, No. 3, 1990, pp. 356-366. Warr, W. A., "Exploiting Molecular Diversity: Small Molecule Libraries for Drug Discovery", Report of Conf rence AΡ 33 held in La Jolla, California, Jan. 23-25, 1995. Westhead, D. R. et al., "A comparison of heuristic search algorithms for molecular docking", Journal of AQ <u>33</u> Computer-Aided Molecular Design, Kluwer Academic Publishers, Vol. 11, 1997, pp. 209-228. Willett, P., "Genetic algorithms in molecular recognition and design", Trends in Biotechnology, Elsevier Science AR <u>33</u> Publishers B.V., Vol. 13, No. 12, December 1995, pp. 516-521. **EXAMINER**

EXAMINER: Initial if reference considered, whether or not citation is in conformance with MPEP 609. Draw line through citation if not in

ATTY. DOCKET NO. 1503.0200006

APPLICATION NO. 09/802

APPLICANT

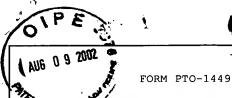
Agrafiotis et al.

ION DISCLOSURE STATEMENT AUG 1 4 7007 GROUP FILING DATE March 12, 2001 2123 TECH CELLICITICS /2900 **U.S. PATENT DOCUMENTS EXAMINER** CLASS DATE NAME SUB-FILING DATE INITIAL DOCUMENT **CLASS** NUMBER AA34 AB34 AC34 AD34 AE34 AF34 Technology Center 2100 AG34 AH34 AI34 **FOREIGN PATENT DOCUMENTS EXAMINER** INITIAL DOCUMENT NUMBER DATE COUNTRY **CLASS** SUB-TRANSLATION **CLASS** AJ34 Yes RECEIVED No AK34 Yes AUG 1 5 2002 No AL34 Yes Technology Center 2100 No Yes AM34 No OTHER (Including Author, Title, Date, Pertinent Pages, etc.) Willett, P. and Winterman, V., "A Comparison of Some Measures for the Determination of Inter-Molecular ΑN Structural Similarity Measures of Inter-Molecular Structural Similarity", Quantitative Structure-Activity <u>34</u> Relationships, VCH, Vol. 5, No. 1, March 1986, pp. 18-25. Zadeh, L. A., "Communication Fuzzy Algorithms", Information and Control, Academic Press, Vol. 12, No. 2, AO <u>34</u> February 1968, pp. 94-102. AP Zadeh, L. A., "Fuzzy Sets", Information and Control, Academic Press, Vol. 8, No. 3, June 1965, pp. 338-353. <u>34</u> AQ Copy of International Search Report issued April 21, 1998 for Appl. No. PCT/US97/20919, 6 pages. 34 AR Copy of International Search Report issued May 13, 1998 for Appl. No. PCT/US97/20918, 7 pages. <u>34</u> **EXAMINER EXAMINER**: Initial if reference considered, whether or not citation is in conformance with MPEP 609. Draw line through citation if not in

conformance and not considered. Include copy of this form with next communication to Applicant.

ATTY. DOCKET NO. 1503.0200006 APPLICATION NO. 09/802,956 APPLICANT Agrafiotis et al.

			CLOSURE STA			Agrafiotis et al. FILING DATE GROUP March 12, 2001 2123					
					U.S. P	ATENT DOCUMENTS					
EXAMINER NITIAL	11105		CUMENT IBER	DATE		NAME	CLASS	SUB- CLASS	FILING DATE		
	AA35	╂									
	AB35 AC35	1		ļ			RECE	IVED			
	AD35	 		_							
	AE35	1		-			AUG 1	2 2002			
	AF35	1	· · · · · · · · · · · · · · · · · · ·			-		Cantar 0100			
	AG35	1					echilology	Center 2100			
	AH35	1	•								
	AI35										
					FOREIGN	N PATENT DOCUMENTS					
EXAMINER INITIAL		DOC	CUMENT NUM	BER	DATE	COUNTRY	CLASS	SUB- CLASS	TRANSLATIO		
	AJ35					RECE	IVED		Y		
	AK35					AUG 1	5 2002		Ye N		
	AL35		<u> </u>			Technology	Center 2100		Ye		
	AM35				1				Ye		
			ОТН	ER (In	cluding Aut	thor, Title, Date, Pertinent Page	s, etc.)				
			l								
MB	AN	<u>35</u>	American Ch	emica	"Analysis of	vorks Applied to Structure-Activity ol. 33., No. 3, 1990, pp. 905-908.	Aliphatic Mol	ecules by Statist	icał and Pattern		
AB	AO	<u>35</u> <u>35</u>	American Ch	et al.,	l Society, Vo "Analysis of ds," Journal	ol. 33., No. 3, 1990, pp. 905-908.	Aliphatic Mol	ecules by Statist	icał and Pattern		
AB			Gasteiger, J. Recognition No. 3, 1993,	et al., Methor pp. 38	"Analysis of ds," Journal 5-394.	ol. 33., No. 3, 1990, pp. 905-908. f the Reactivity of Single Bonds in	Aliphatic Moler Science, An	ecules by Statist erican Chemica	ical and Pattern I Society, Vol. 3		
AB	AO	<u>35</u>	Gasteiger, J. Recognition No. 3, 1993, Guez, A. and integrated me	et al., Methodopp. 38	"Analysis of ds," Journal 5-394. , I., "Neural I	ol. 33., No. 3, 1990, pp. 905-908. If the Reactivity of Single Bonds in of Chemical Information Computer	Aliphatic Moler Science, Am al laboratory coublishers B.V.	ecules by Statist erican Chemica emputing with ap Vol. 248, 1996,	ical and Pattern I Society, Vol. 3 oplication to pp. 73-90.		
AB	AO	<u>35</u>	Gasteiger, J. Recognition No. 3, 1993, Guez, A. and integrated modern of the Ridder, D. de Ridder, D.	et al., Methor pp. 38 I Nevo conitorin	"Analysis of ds," Journal 5-394. , I., "Neural ing," Clinica (ol. 33., No. 3, 1990, pp. 905-908. If the Reactivity of Single Bonds in of Chemical Information Computer Computer Computer Computer Chemical Acta, Elsevier Science P	Aliphatic Moler Science, Amal laboratory coublishers B.V.	ecules by Statist erican Chemica emputing with ap Vol. 248, 1996, hemistry, Spring	ical and Pattern I Society, Vol. 3 pplication to pp. 73-90. per-Verlag, Vol.		



ATTY. DOCKET NO. APPLICATION NO. 1503.0200006 09/802,956

APPLICANT Agrafiotis et al. GROUP

TRATE TRANS	ORMATTO	N DT	SCLOSURE ST	атеме	NT	Ag	rafiotis et	al.				
o TRATA	TRANSFORMATION DISCLOSURE STATEMENT							FILING DATE GROUP March 12, 2001 2123				
· · · · · · · · · · · · · · · · · · ·					U.S. F		T DOCUMENTS					
EXAMINER INITIAL			DOCUMENT NUMBER		DATE		NAME		CLASS	SUB- CLASS	FILING DATE	
	AA36						· · · · · · · · · · · · · · · · · · ·					
	AB36											
	AC36							R	ECEI	VED		
	AD36											
	AE36								AUG 1 2	ZUUZ		
	AF36	<u> </u>				_		Tech	holoov C	enter 2100		
	AG36			_		ļ		1001	riology C	CIRCI Z I U		
	AH36	-				 					_	
	Al36								<u></u>			
EVANNED	1	1			FOREIG	N PAT	ENT DOCUMEN	ITS	r		1	
EXAMINER INITIAL		DO	CUMENT NUM	/BER	DATE	· · · · · · · · · · · · · · · · · · ·	COUNTRY	PEC	class EIVED	SUB- CLASS	TRANSLATION	
	AJ36							1120		ļ	Yes No	
	AK36							AUG 1	5 2002		Yes	
	71/30										No	
	AL36							technolog	y Center 2	100	Yes No	
	AM36										Yes	
		1	OTL	IED (In	oludina Aut	thor T	itle, Date, Perti	nont Pages, etc			No.	
AB	AN	<u>36</u>	Kim, H. et a	l., "Self Syster	-Organized	Distribi <i>Artificia</i>	uted Networks fo al Neural Networ	or Learning High	ly Nonlinear			
	AO	<u>36</u>	Pal, N.R. an Reduction,"	d Eluri, IEEE 7	, V.K., "Two Transactions	Efficier	nt Connectionist ural Networks, II	Schemes for St EEE, Vol 9, No.	tructure Pres 6, Novembe	erving Dimer r 1998, pp. 1	nsionality 142-1154.	
	AP	<u>36</u>	Domine, D. Chemometri	Domine, D. et al., "Non-Linear Mapping for Structure-Activity and Structure-Property Modelling," Journal of Chemometrics, John Wiley & Sons, Ltd., Vol. 7, No. 4, July-August 1993, pp. 227-242.								
	AQ	<u>36</u>	Hosenpud, J. et al., "The Effect of Transplant Center Volume on Cardiac Transplant: A Report of the United Network for Organ Sharing Scientific Registry," <i>Journal of the American Medical Association</i> , American Medical Association, Vol. 271, No. 23, June 15, 1994, pp. 1844-1849.									
1	AR	<u>36</u>	English-lang Date of publ	juage A ication	Abstract of E of applicatio	uropea on).	n Patent No. 0 3	355 628, printed	from Dialog	File No. 351(February, 1990 -	
EXAMINER	1/		118	····				Tr	DATE GONS	Ø ERED		

EXAMINER Januelly works

DATE CONSIDERED